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Title: Critical Experiment Benchmark Results using MCNP6.2 Unstructured Mesh

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Critical Experiment Benchmark Results using MCNP6.2 Unstructured Mesh (UM)

Introduction

The purpose of this report is to document the results of five critical experiment benchmarks modeled using the unstructured mesh (UM) geometry capability in MCNP®[1] code, version 6.2, Reference (1). LANL currently has a vast critical experiment benchmark library with over 1100 cases, modeled using constructive solid geometry (CSG) and packaged with Whisper-1.1, Reference (2). Validation efforts for the purposes of nuclear criticality safety typically focus on benchmark libraries built using CSG models. Results of UM geometry models are compared with CSG results and the critical experiment k-effective from the ICSBEP handbook, Reference (3). All computed k-effective results in this study are well within 1% of the experimental result.

The following experiments are modeled for this study:

HEU-MET-FAST-001:	Godiva, a bare, fast, spherical assembly of highly enriched uranium metal, 94% ^{235}U.
HEU-MET-FAST-007-037:	Highly enriched uranium metal slabs moderated with polyethylene and reflected with polyethylene.
IEU-MET-FAST-007:	Big Ten, a large, mixed-uranium cylindrical core with 10% average ^{235}U enrichment, surrounded by a thick ^{238}U reflector.
PU-MET-FAST-022:	A bare, fast, spherical assembly of delta-phase plutonium metal, 98% ^{239}Pu.
PU-SOL-THERM-001-001:	A water-reflected 11.5-inch diameter sphere of plutonium nitrate solution.

The MCNP® UM geometry capability is a relatively recent development, Reference (4), and its use for modeling criticality problems is not yet widely adopted. This report discusses important considerations when modeling criticality problems using UM geometry and proposes engineering best practices they are employed to avoid potential issues.

While the use of UM geometry in MCNP6 is a relatively new feature, it has primarily been employed in practical applications for doing shielding and dose calculations, i.e. fixed source problems. The preservation of mass and volume when moving from CSG to UM geometry is an essential concern and the importance of this cannot be overstated when employing UM for criticality problems. It is possible to generate a mesh, which for most purposes reflects the geometry adequately and yet does not properly preserve mass and/or volume to the degree necessary for correct criticality calculation leading to incorrect k-effective results. In criticality calculations, even slight increases or decreases in fissile/fissionable mass can lead to significant differences in reactivity. For this reason, when modeling geometries using UM for criticality problems practitioners must always check to see that mass and volume are within acceptable tolerances. The next section discusses details of creating meshes for use with UM in MCNP6 and

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gives guidance learned by those with experience using UM with MCNP6. This report, with future similar studies, is an effort to begin considering validation using criticality safety benchmark experiments. It cannot, and is not intended to, replace site-wide nuclear criticality safety validation guidance, which must be considered by the criticality safety practitioner in the context of the process analysis requirement in ANSI/ANS-8.1 [Reference (5)]. For programs that follow ANSI/ANS-8.24 [Reference (6)], the method of analysis in a criticality safety evaluation must be the same method covered by validation for a criticality safety program. It is advisable for programs to consider whether it is appropriate to use a collection of CSG benchmarks to conduct validation for UM cases and vice-versa. It is useful to note, however, that for the benchmarks presented in this report careful choice of UM methods leads to good agreement (much less than 1% calculational bias) between CSG, UM, and the benchmark experiment k-effective eigenvalue. A simple summary of results is presented in Table 1. Detailed descriptions of the experiments, models, techniques, and results are presented in subsequent sections.

Table 1. Summary of Criticality Results Comparing Experimental, Reference CSG k-effective values and k-effective values using MCNP6.2 UM

Benchmark	Experiment k-effective	Experiment uncertainty	MCNP6.2 CSG k-effective	MCNP6.2 CSG uncertainty	MCNP6.2 UM k-effective	MCNP6.2 UM uncertainty
HEU-MET-FAST-001	1.0000	0.10%	1.0000	0.01%	0.9984	0.01%
HEU-MET-FAST-007-037	0.9988	0.08%	1.0018	0.01%	1.0017	0.01%
IEU-MET-FAST-007	1.0045	0.07%	1.0044	0.01%	1.0040	0.01%
PU-MET-FAST-022	1.0000	0.21%	0.9983	0.01%	0.9960	0.06%
PU-SOL-THERM-001-001	1.0000	0.50%	1.0058	0.01%	1.0030	0.08%

General Methodology for Construction of UM Models

The general method followed for the benchmarks in this study involves the use of the Attila4MC package [Reference (7)] with the following steps:

1.) Construction of a solid geometry using SpaceClaim [Reference (8)],
2.) Importation of the solid geometry into the Attila4MC project,
3.) Creation of the mesh using Attila4MC,
4.) Specification of a calculation using the Attila4MC graphical user interface,
5.) Modification of the MCNP6.2 input file to specify kcode parameters,
6.) Execution of MCNP6.2 kcode calculation passing statistical and convergence checks,
7.) Comparison of calculated k-effective result with experiment result, and
8.) Conversion of .eeout to .vtk using a script [Reference (9)] for visualization with Paraview [Reference (10)].

A different method for obtaining an unstructured mesh geometry for MCNP6.2 UM uses Abaqus [Reference (11)]. Although this study does not use the Abaqus method, the engineering best practices offered should apply equally well, regardless of whether the model construction method uses Attila4MC or Abaqus.

In the descriptions given below, details regarding the specific models are stated primarily in the Attila4MC terminology of node points (vertices for 1st order elements), sides (faces) and elements. In MCNP UM terminology, vertices are equivalent to node points for 1st order elements, faces are equivalent to sides. For 2nd order elements vertices and mid-points between vertices are equivalent to node points. Elements are known as cells in Attila4MC, but such terminology is not used in this study to avoid confusion with CSG cells.

In all models where there is curvature, automatic curvature refinement in Attila4MC is used, wherein the feature will locally reduce the element edge length to capture surface curvature. In addition, "refine anisotropically" is selected to refine elements only in the curvature direction. Other directions are determined by the maximum edge length setting for that region.

All calculations in this study use 1st order tetrahedral elements. MCNP6.2 allows UM geometries using 1st and 2nd order elements, which may be tetrahedral, pentahedral, or hexahedral. 1st order elements have nodes only at vertices, 2nd order elements have nodes at vertices and on edges (at mid-points) between vertices.

All kcode calculations were run with 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles and ensuring both convergence of k-effective and the fission source distribution. Results for both CSG and UM were within 1% of the experiment value.

Benchmark Descriptions, MCNP6 Models and Results

HEU-MET-FAST-001 was performed at Los Alamos in the 1950's to determine the critical mass of 94% ^{235}U, Godiva consisted of two identical sets of nested oralloy hemispheres, a photo from the handbook is shown in Figure 1. The upper set of hemispheres was supported by a 0.015-inch thick diaphragm of stainless steel. The lower set of hemispheres rested on an aluminum cylinder. The lower stack was raised remotely to contact the steel diaphragm.

The benchmark specifications of Godiva for an experimental k-effective of 1.00 with experimental uncertainty of 0.001 consists of a bare sphere of 93.71 wt% ^{235}U with a diameter of 8.7407 cm and a mass of 52.42 kg. The uranium metal density is 18.74 g/cm^3 with 1.02 wt% ^{234}U and 5.27 wt% ^{238}U.

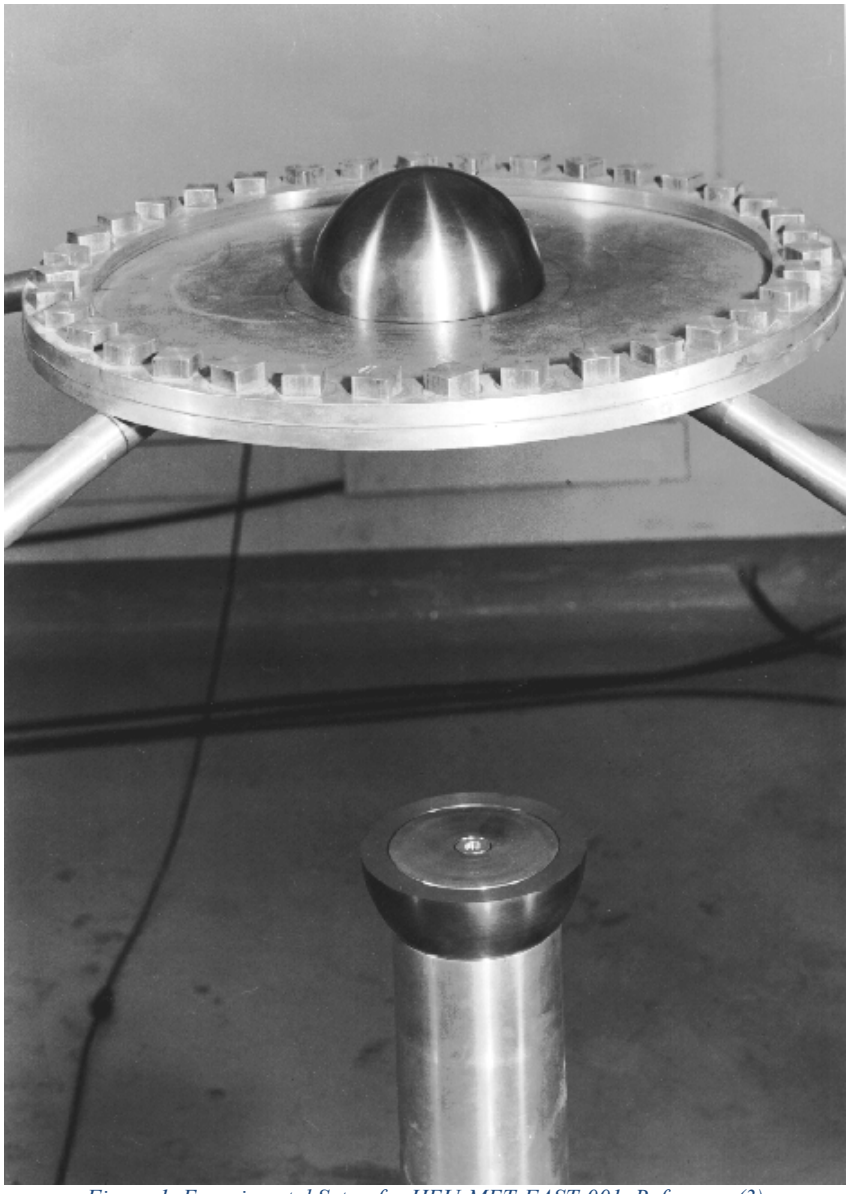

Figure 1. Experimental Setup for HEU-MET-FAST-001, Reference (3)

HMF-001 is simple to model using the CSG method and consists of one sphere with a radius of 8.741 cm. A geometry illustration from MCNP6.2 is shown in Figure 2. The CSG model kcode calculation using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00000 with a standard deviation of 0.00008.

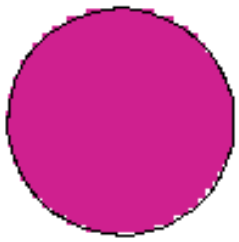

Figure 2. MCNP6.2 Illustration of HEU-MET-FAST-001

The MCNP6.2 UM model is built by first constructing a solid geometry in SpaceClaim, the solid geometry is imported into Attila4MC and a mesh is generated. There are several mesh options available, including a specification for the maximum edge length. Figures 3 and 4 show results of the mesh depending on the choice of maximum edge length ranging from 1 cm to 12 cm to illustrate how various choices effect the mesh. There exists a tradeoff between specifying an edge length small enough to provide enough geometry detail and one not too small to result in unnecessary detail with regard to number of cells in the mesh. For this problem, choosing a maximum edge length of 1 to 2 cm appears to be a good balance between specifying enough detail and maintaining enough efficiency for an adequate k-effective calculation in MCNP6.2 to obtain a result well-within 1% of the experiment result.

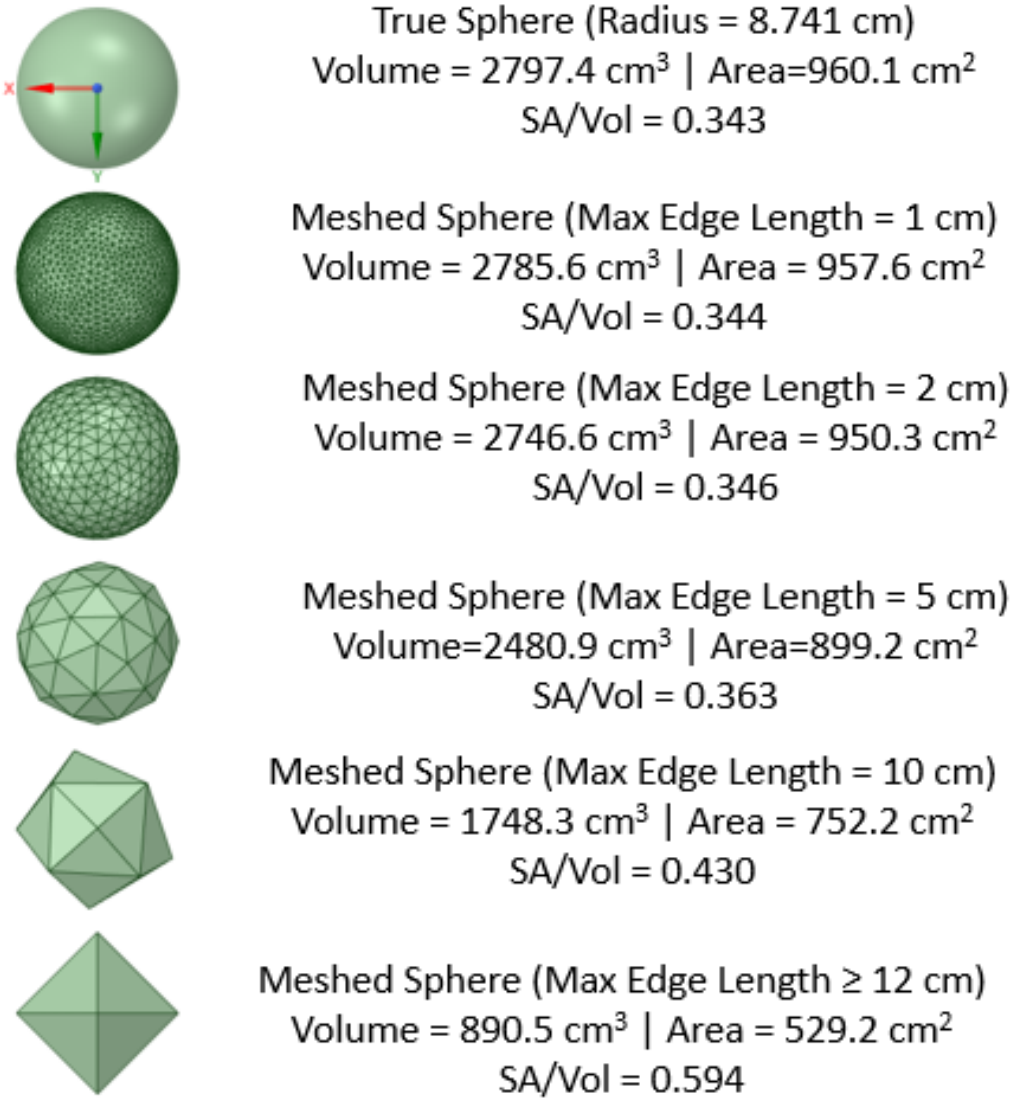

Figure 3. Mesh representations of HEU-MET-FAST-001 as a function of maximum edge length

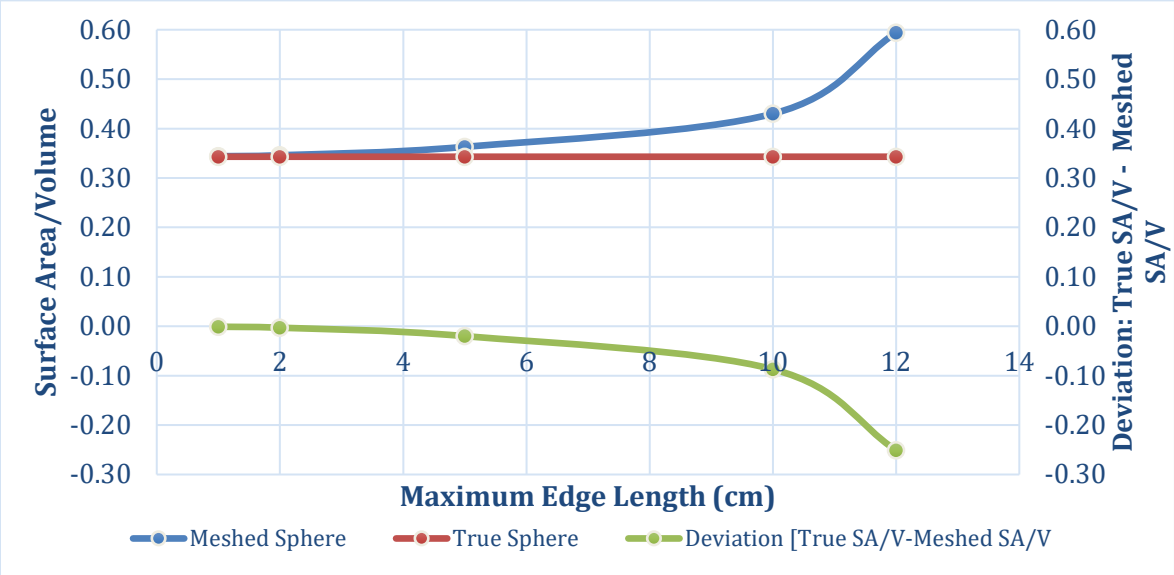

Figure 4.Surface Area-to-Volume Ratio of True Sphere and Meshed Spheres for HEU-MET-FAST-001

Once the mesh is generated, it is used to build a calculation in Attila4MC. After specifying calculation parameters such as materials, Attila4MC creates an Abaqus mesh file and an MCNP6 input file. The MCNP6.2 UM kcode calculation using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles result is 0.99837 with a standard deviation of 0.00009. Figure 5 shows a cross section illustration of the results for element-average neutron flux when using a mesh with a maximum edge length of 2 cm resulting in an UM with a total of 762 node points (vertices), 668 sides (faces), and 3278 tetrahedral elements. Figure 6 shows the MCNP6.2 UM results when using different maximum edge length specifications.

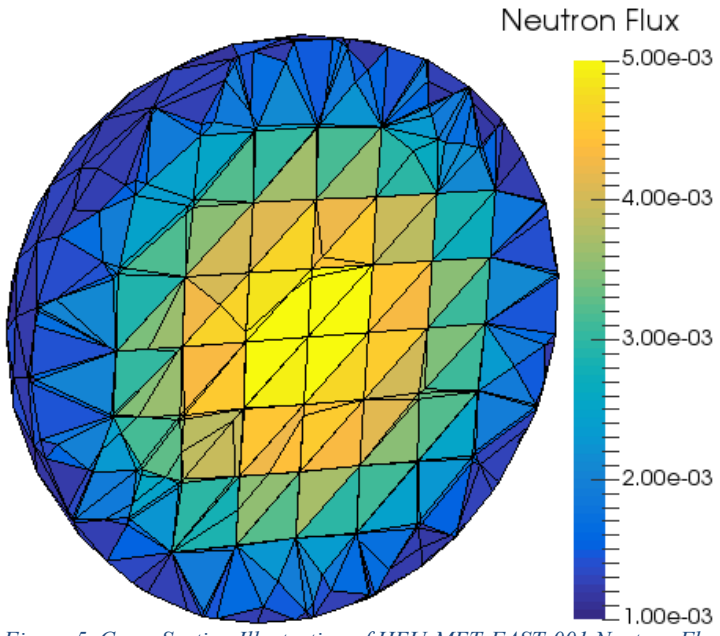

Figure 5. Cross Section Illustration of HEU-MET-FAST-001 Neutron Flux

Another technique relevant to UM calculations involves a mass correction applied to the model. The actual volume for a specific part is compared to the volume of the meshed part. As can be

seen in Figure 3, the volume of the true sphere is ~2797 cm^3. The volume of the sphere decreases when the maximum edge length is increased. A mass correction is performed by applying a density factor equal to the ratio of the true volume to the meshed volume. The results in Figure 6 show the difference in k-effective results for a part with the same mass but increased density as a function of volume differences stemming from too large a maximum edge length as well as a set of curves where no density adjustment was made. As is expected in the non-corrected cases, as the volume and consequently the critical mass representation goes down so does the calculated k-effective value. In the density-adjusted cases, the critical mass was maintained, but as the mesh shape moved farther away from spherical the calculated k effective value increased even more than the magnitude of equivalent decrease associated with the reduced mass. Although the above results demonstrate that the density adjustment technique tends to be conservative, it is recommended that it be used with caution. Furthermore, it is recommended that in addition to volume preservation the surface area to volume ratio should also be considered when constructing a mesh representation of a critical assembly. It appears for this problem to get a calculated k-effective result within 1% of the experimental k-effective value of 1.000 an adequate maximum edge length is around 1-2 cm. Based on this result and examining the parameters included in Figure 3 a recommended rule of thumb for mesh quality is that the total meshed volume of the active elements of a model agree with the analytical volume to within at least 2% and that the surface area to volume ratio agree to within 1%.

Figure 6 also provides results of an independent check to the MCNP6.2 results calculated using the Attila deterministic k eigenvalue solver. The deterministic calculations used the Radion5 general-purpose reactor analysis multi-group cross section library with 30 neutron and 25 gamma groups. The Attila calculations used the S_{12} Triangular Chebychev Legendre angular quadrature set with a P_3 Galerkin scattering treatment. The deterministic results support the same conclusion as the MCNP6.2 calculations.

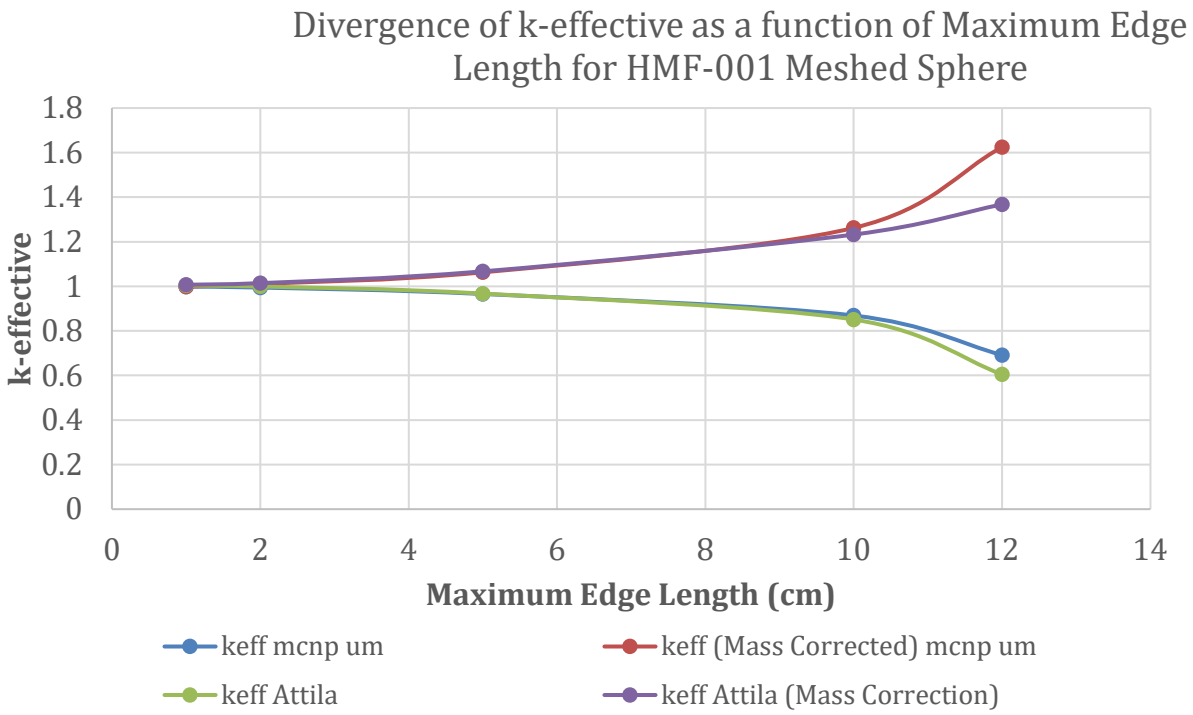

Figure 6. K-effective as a function of maximum edge length for HEU-MET-FAST-001

HEU-MET-FAST-007-037 is one of forty-three critical experiments involving moderated slabs of highly enriched uranium metal performed at Oak Ridge National Laboratory in 1967. In this case, there is six inches of polyethylene reflection in the experiment and polyethylene is interleaved between six 93.15 wt% ^{235}U slabs. The experiment was performed on split table apparatus in which half of the assembly was placed on a moveable bench and half of the assembly was placed on a stationary bench. The two halves were brought together with essentially no gap between the halves. The critical parameters for case 37 are a uranium metal mass of 28.738 kg, plastic mass of 0.6716 kg, assembly height of 7.120 cm and six cells for experimental k-effective of 0.9988 and experimental uncertainty of 0.0008. An example of the experimental series assembly from the handbook is shown in Figure 7.

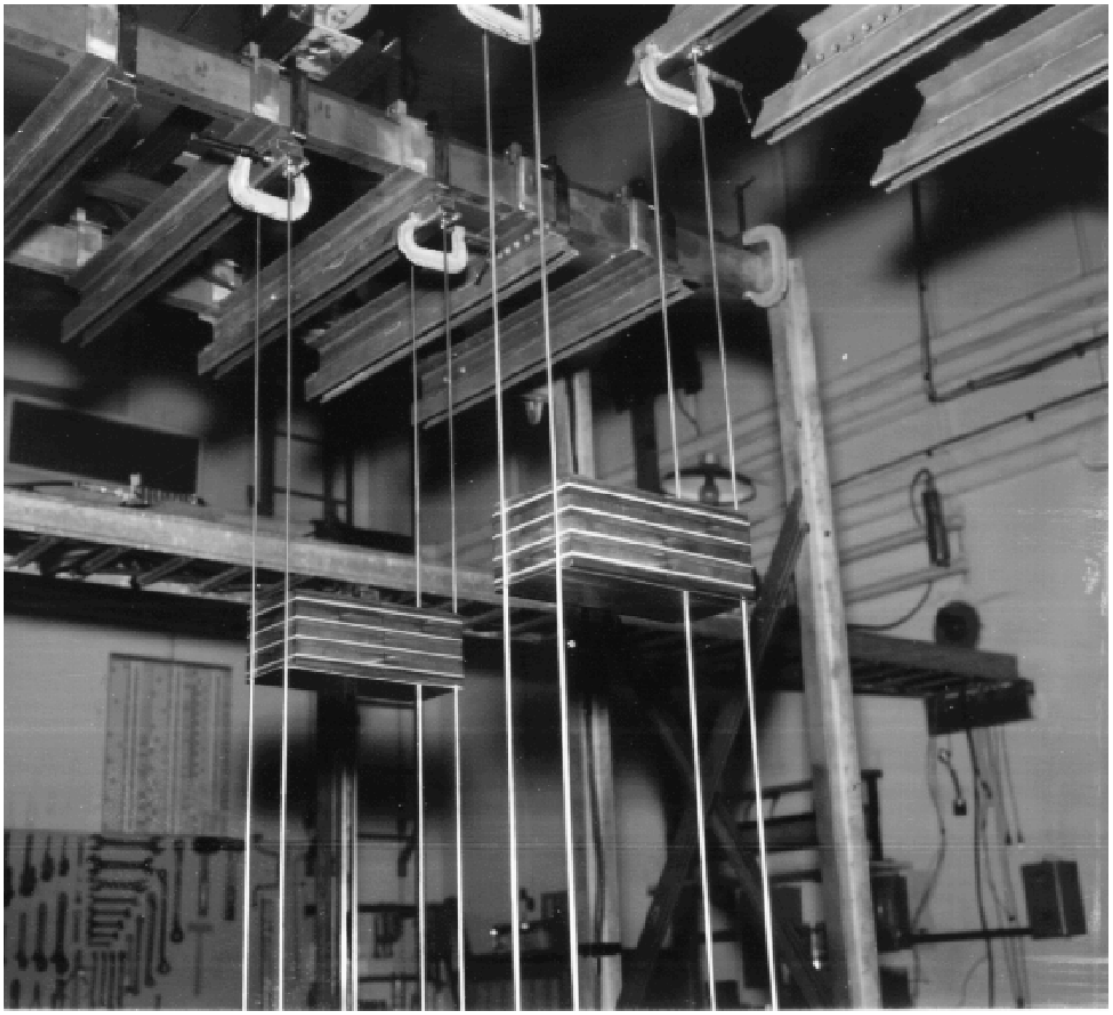

Figure 7. HEU-MET-FAST-037 Experimental Assembly Area from Reference (3).

A geometry illustration from MCNP6.2 is shown in Figure 8. The CSG model kcode calculation using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles result is 1.00182 with a standard deviation of 0.00012.

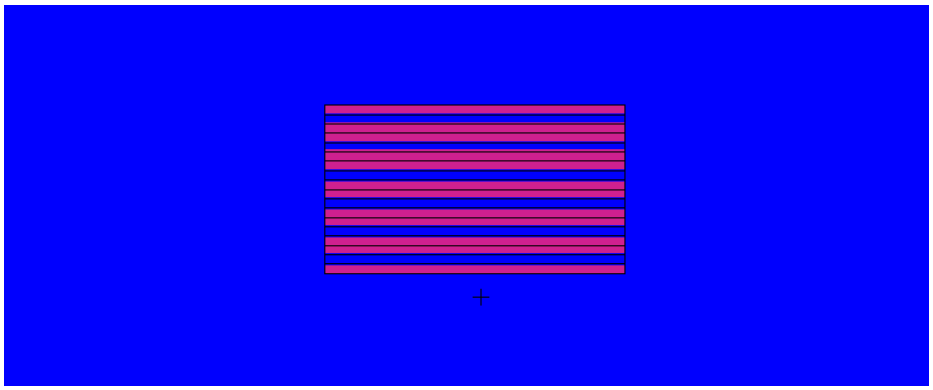

Figure 8. MCNP6.2 Illustration of HEU-MET-FAST-007 case 37. Magenta=HEU, Blue & Yellow=polyethylene

The MCNP6.2 UM is built by first constructing a solid geometry in SpaceClaim, the solid geometry is imported into Attila4MC and a mesh is generated. The solid model is shown in Figure 9.

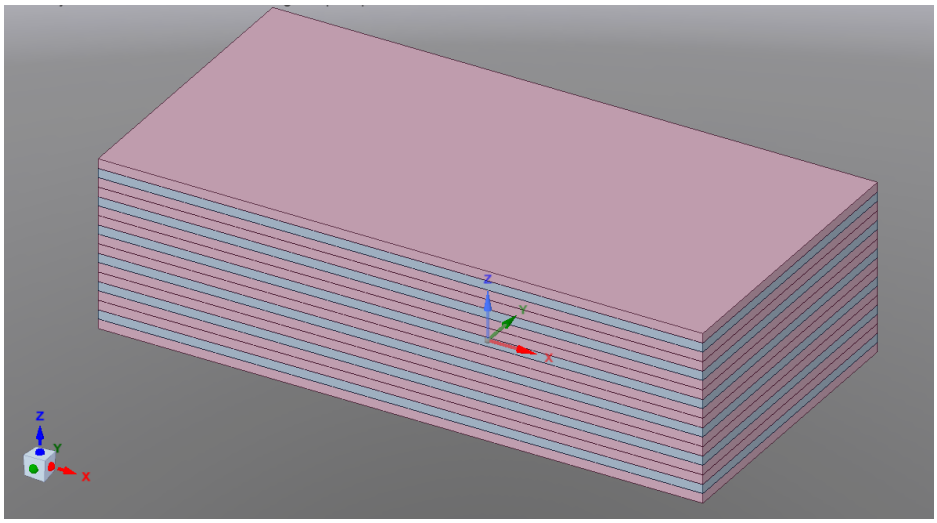

Figure 9. Illustration of HEU-MET-FAST-007 Solid Geometry

There are several mesh options available, including a specification for the maximum edge length. There exists a tradeoff between specifying an edge length small enough to provide enough geometry detail and one not too small to result in unnecessary detail with over-conservatism with regard to number of cells in the mesh. For this problem, choosing a maximum edge length of 6.35 cm appears to be a good balance between specifying enough detail and maintaining enough efficiency for an adequate k-effective calculation in MCNP6.2 to obtain a k-effective result within 1% of the experiment value. In this case, the advanced features of curvature refinement and refine anisotropically were not selected because this problem does not have curvature. The resulting mesh has a total of 1419 node points (vertices), 1754 sides (faces), and 6880 tetrahedral elements. The mesh connectivity is shown in Figure 10 and includes a bounding box around the fuel plates with moderator.

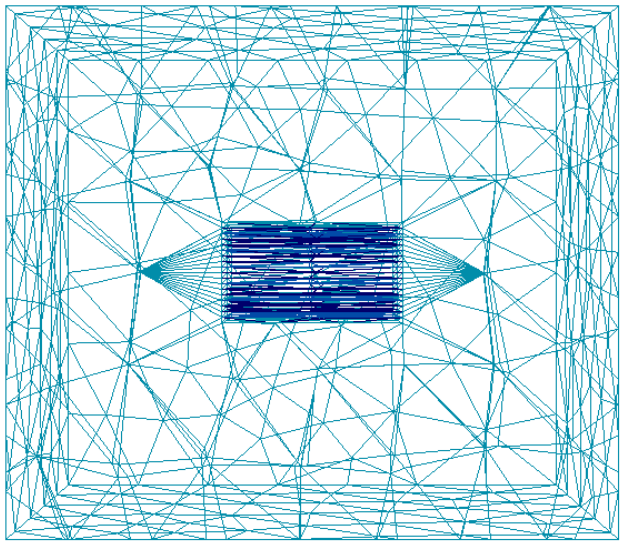

Figure 10. Illustration of HEU-MET-FAST-037-007 Mesh

The MCNP6.2 UM kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00166 with a standard deviation of 0.00011. Figure 11 shows a cross section illustration of the neutron element-average flux results.

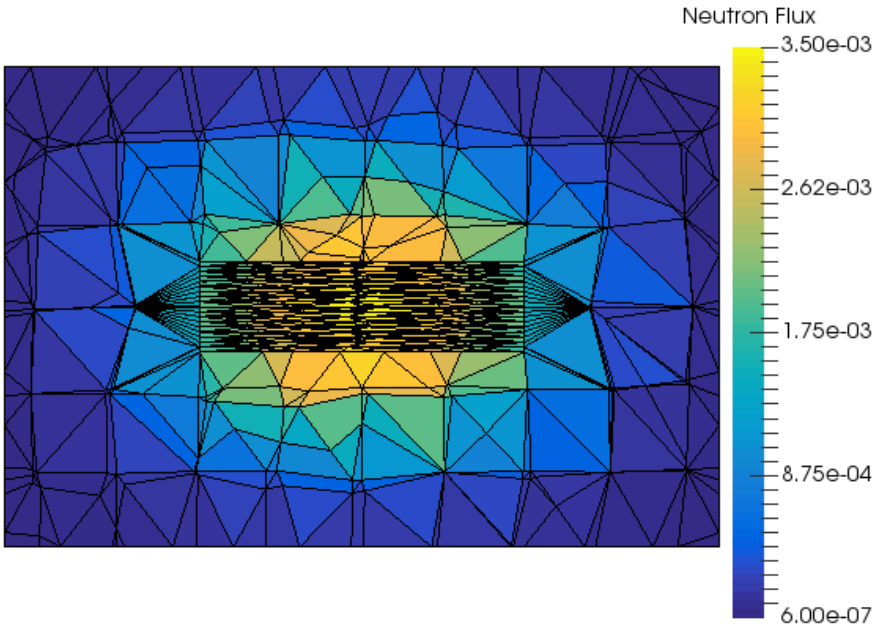

Figure 11. Cross Section Illustration of MCNP6.2 Neutron Flux Results

IEU-MET-FAST-007 is also referred to as Big Ten, a large, mixed-uranium cylindrical core with 10% average ^{235}U enrichment, surrounded by a thick ^{238}U reflector. The total uranium mass is 10 metric tons. A schematic drawing of Big Ten experiment is shown in Figure 12. A detailed analysis of using MCNP UM for Big Ten can be found in Reference 12.

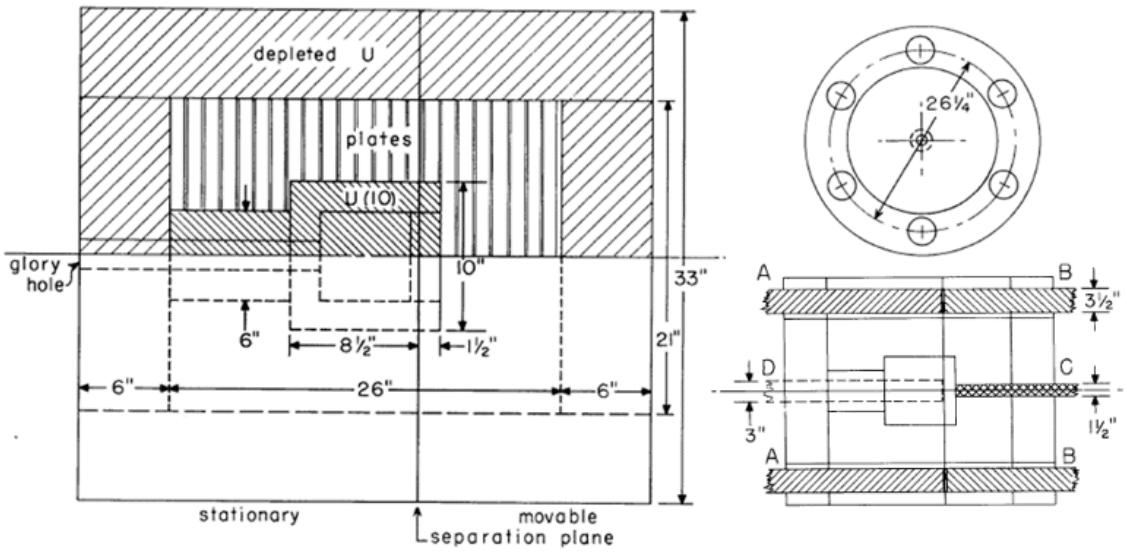

Figure 12. Cross Section Illustration of the Big Ten Critical Assembly, Reference (3)

The CSG model illustration from MCNP6 is shown in Figure 13. The CSG model kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00435 with a standard deviation of 0.00007.

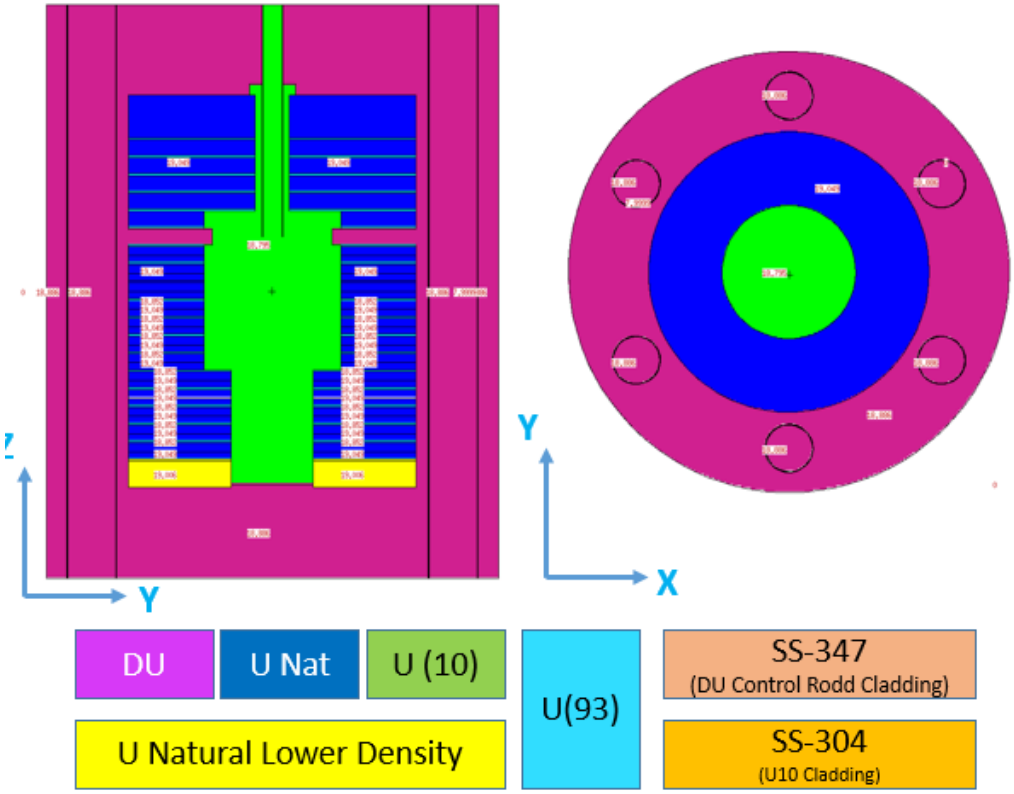

Figure 13. Cross Section Illustration of Big Ten CSG Model with MCNP6.2

Several meshing techniques were used to generate an optimized mesh, such as pre-faceting the cylindrical rods into a 20-sided polyhedron, curvature refinement, and anisotropic mesh refinement. A global mesh size of 5 cm was found to be an adequate balance between fine enough mesh to obtain a result within 1% of the experiment value while being coarse enough so as not to add detail increasing computational time and memory requirements without commensurate benefit for this problem. Part specific maximum edge length of 4 cm for the DU control rods and 1.5 cm for the 10% enriched uranium rod located on axis. Beyond these parameters, two separate approaches were taken to construct a mesh model of Big Ten: first a direct analog to the CSG model was constructed where each thin fuel plate was modeled explicitly and a second model was constructed where the fuel plates were homogenized into top middle and bottom sections based on radial similarity of the annular plate geometry. Further details are discussed in Reference 12. A cross section illustration of the solid geometry for the explicit model is shown in Figure 14 with its corresponding mesh connectivity shown in Figure 15 with a total of 285,322 tetrahedral elements with 49,382 node points (vertices) and 71,206 sides (faces). The MCNP6.2 UM kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00400 with a standard deviation of 0.00007. Figure 16 shows the mesh model with the homogenized fuel plates, which has 127,326 tetrahedral elements, which is over 55% lower element count than the explicit model which would therefore require less than half the amount

memory and time to estimate the k-effective value in MCNP6.2. The simplified homogenized version of this model produced a k-effective value of 1.00025±0.00007.

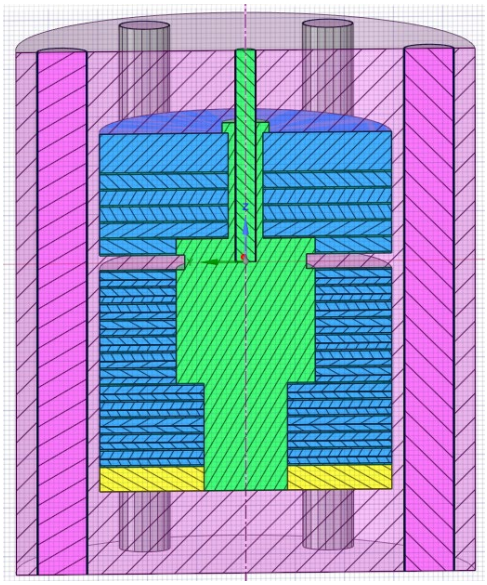

Figure 14. Cross Section Illustration of Big Ten Solid Geometry

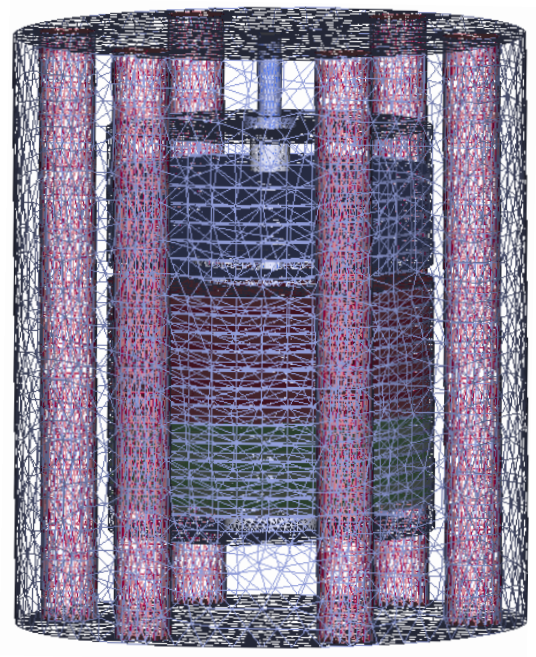

Figure 15. Illustration of Big Ten Mesh Model with Fuel Plates Modeled Explicitly

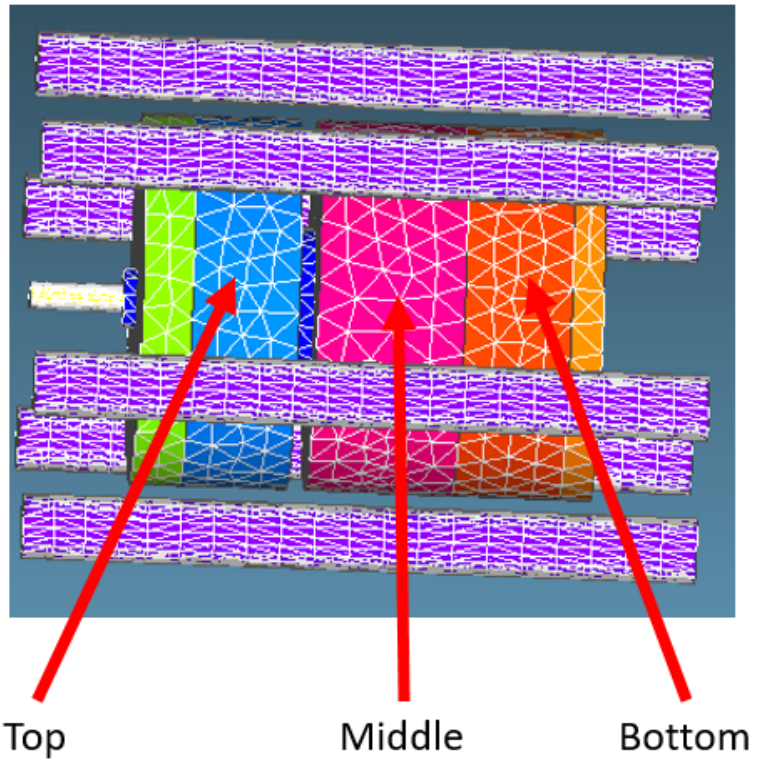

Figure 16. Illustration of Big Ten Mesh Model with Homogenized Fuel Plates

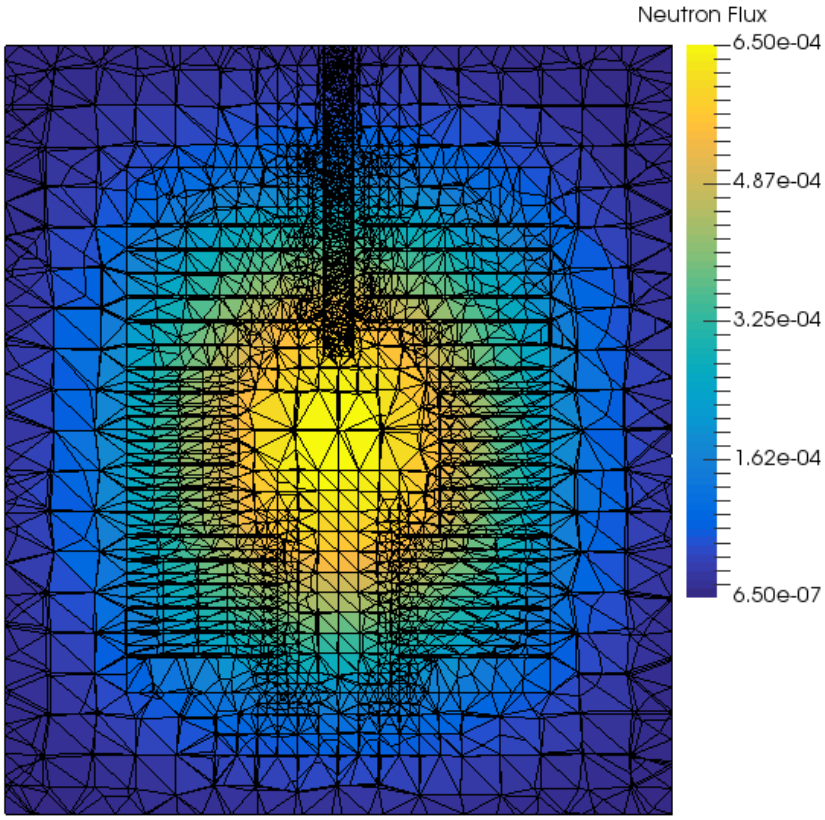

Figure 17. Cross Section Illustration of Average Neutron Flux Results for IEU-MET-FAST-007

PU-MET-FAST-022 is a bare, fast, spherical assembly of delta-phase plutonium metal, 98% ^{239}Pu. An illustration of the experiment is shown in Figure 18.

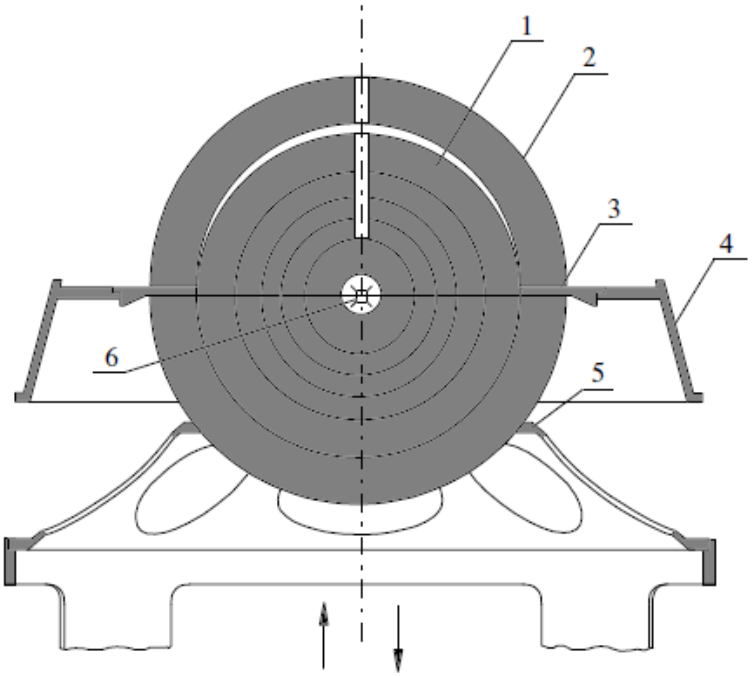

Figure 18. Cross Section Illustration of PMF022. 1-lower core; 2-upper core; 3-steel diaphragm; 4-upper support; 5-lower support; 6-neutron source, Reference (3)

A geometry illustration from MCNP6.2 is shown in Figure 19. The CSG model kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 0.99830 with a standard deviation of 0.00008.

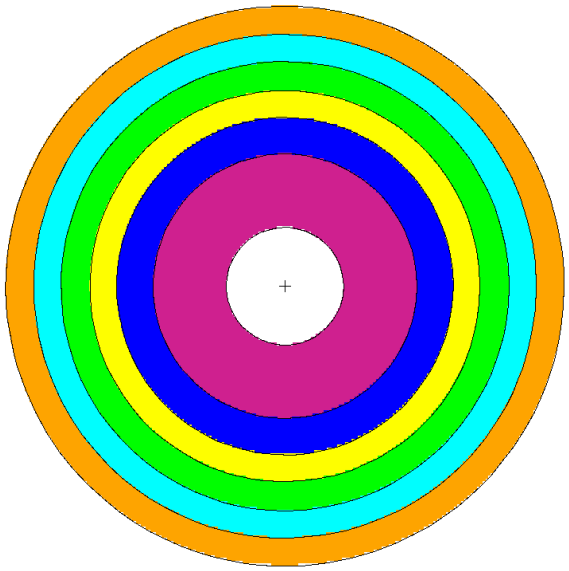

Figure 19. MCNP6.2 Illustration of PU-MET-FAST-022 CSG Model

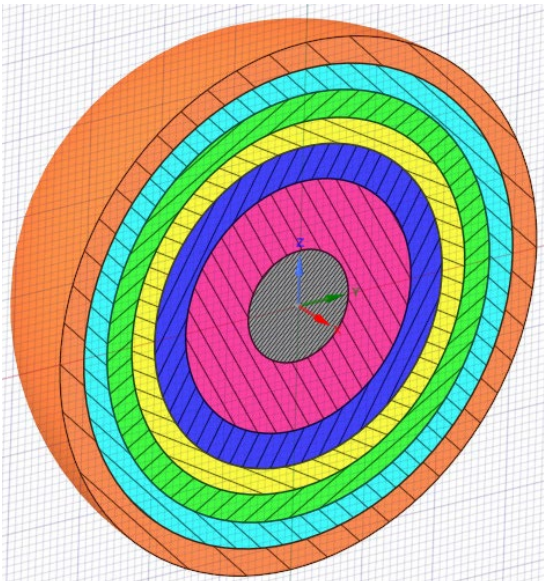

Figure 20. Cross Section Illustration of PU-MET-FAST-022 Solid Geometry

The mesh is generated using a global mesh maximum edge length of 1 cm using curvature refinement and anisotropic refinement. The following is a summary of the statistics for the UM used for the PU-MET-FAST-022 benchmark: total number of 12758 node points (vertices), 10496 sides (faces), and tetrahedral elements 70532. The mesh connectivity is shown in Figure 20.

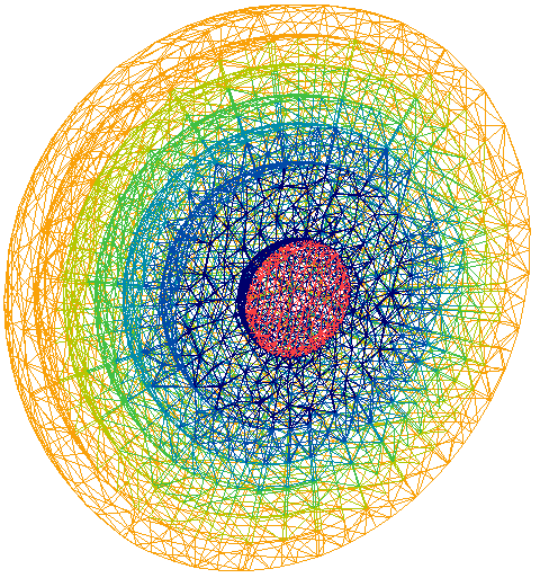

Figure 21. Cross Section Illustration of PU-MET-FAST-022 Mesh

The MCNP6.2 UM kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 0.99598 with a standard deviation of 0.00063. Element-average track-length neutron flux estimates are shown in Figure 21.

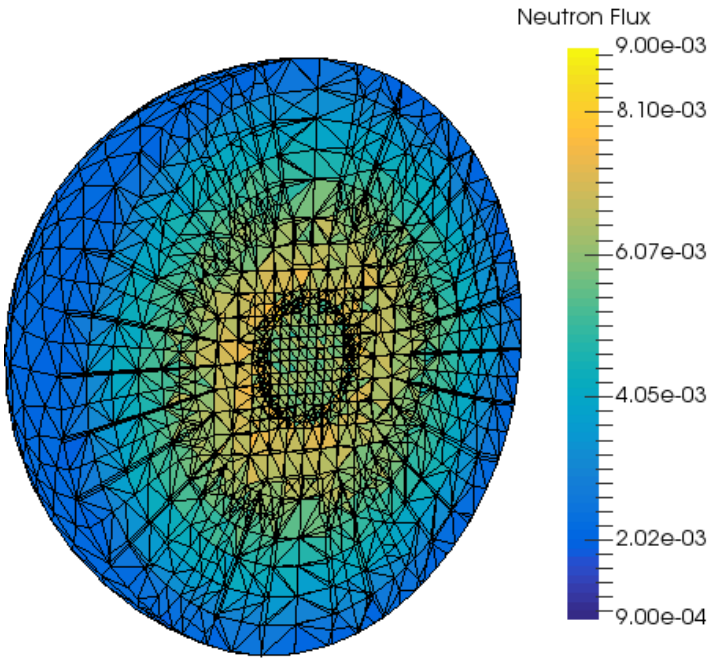

Figure 22. Cross Section Illustration of Neutron Flux Results for PU-MET-FAST-022

PU-SOL-THERM-001 is a water-reflected 11.5-inch diameter sphere of plutonium nitrate solution in a stainless steel tank. The concentration of plutonium in the solution is 73 g/L with nitric acid molarity of 0.2 N. The density of the solution is 1.130 g/cm^3 with a total critical volume of solution of 12.95 L. An illustration of the experiment is shown in Figure 22.

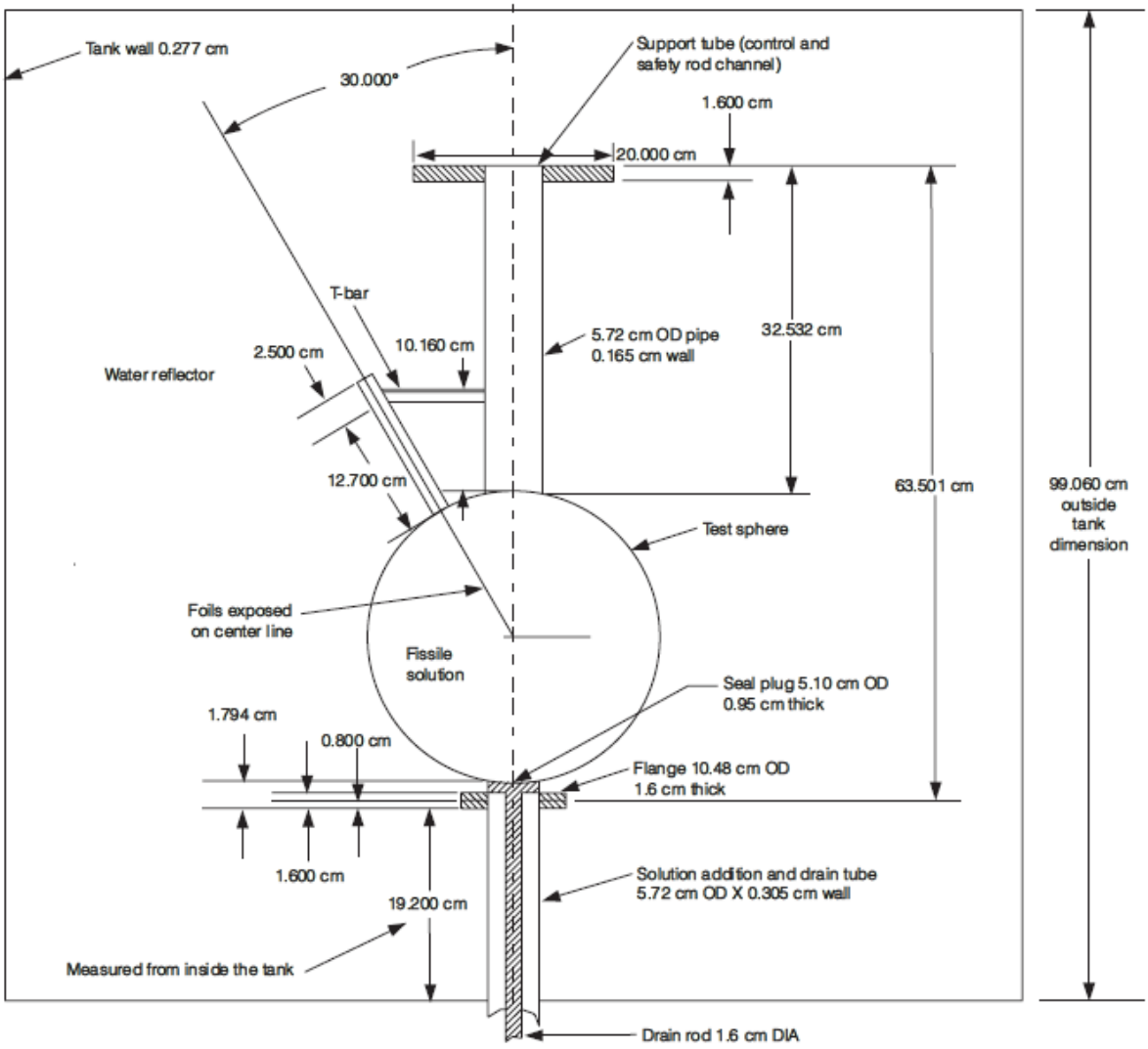

Figure 23. Illustration of PU-SOL-THERM-001-001

A geometry illustration from MCNP6.2 is shown in Figure 24. The CSG model kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00578 with a standard deviation of 0.00013. The solid geometry is shown in Figure 25.

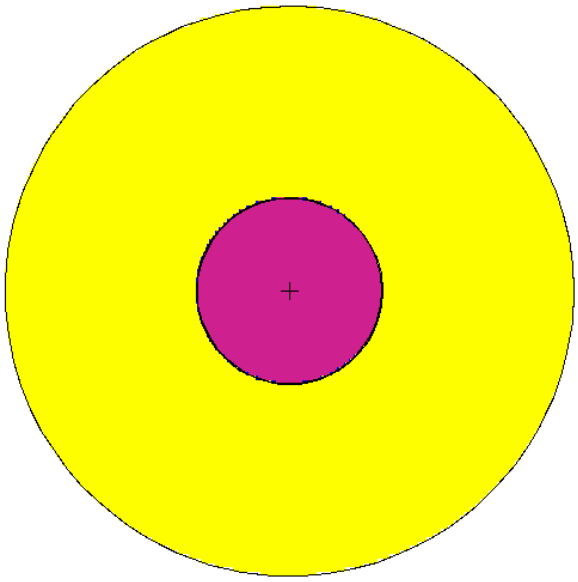

Figure 24. MCNP6.2 Illustration of CSG PU-SOL-THERM-001-001 Model

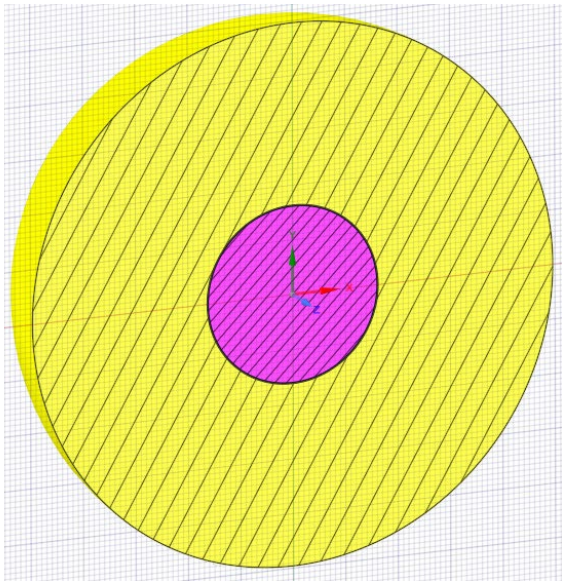

Figure 25. Cross Section Illustration of PU-SOL-THERM-001-001 Solid Geometry Model

The mesh is generated using a global mesh maximum edge length of 5 cm using curvature refinement and anisotropic refinement. The following is a summary of the statistics for the UM used for the PU-SOL-THERM-001-001 benchmark: total number of 6934 node points (vertices), 4290 sides (faces), and tetrahedral elements 38357. The mesh connectivity is shown in Figure 26.

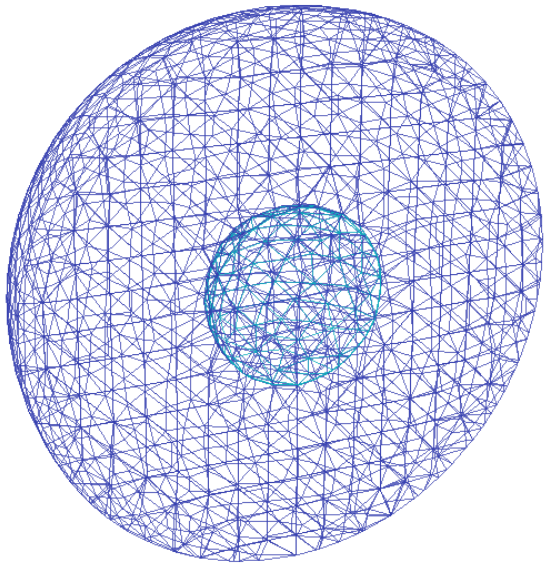

Figure 26. Cross Section Illustration of PU-SOL-THERM-001-001 Mesh Model

The MCNP6.2 UM kcode calculation result using 100,000 neutrons per cycle, skipping 100 cycles with 500 active cycles is 1.00299 with a standard deviation of 0.00081. Element-average track-length neutron flux estimates are shown in Figure 27.

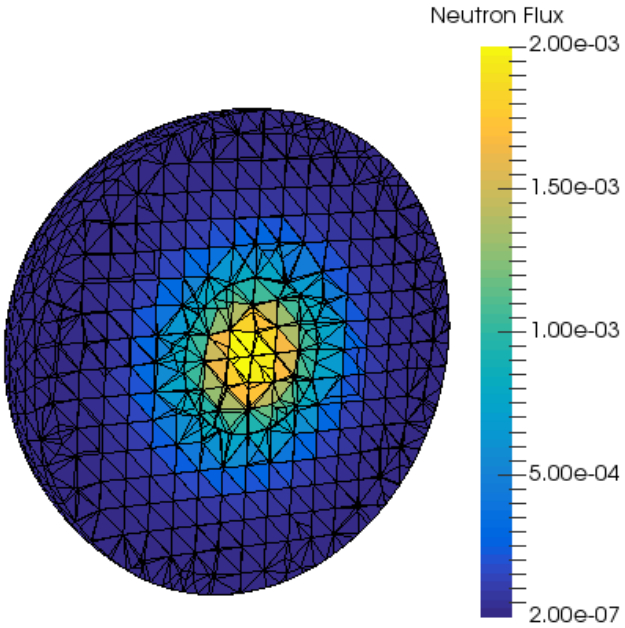

Figure 27. Cross Section Illustration of MCNP6.2 Neutron Flux Results

Conclusions and Guidance on UM Construction Techniques

It has been shown in this report that it is possible to model critical assemblies with the MCNP6.2 UM method to obtain k-effective values that are within one half of a percent of experimental values so long as due care is applied to mesh quality, especially in preserving both the mass and shape of the active elements. Table 2 shows the percent differences obtained for calculated k-effective values relative to experimentally derived benchmark values for MCNP6.2 CSG and

UM geometry descriptions with the same kcode specification. In both cases, the differences to experiment are well below 1%. It has also been shown that the calculated k-effective values can easily be incorrect if proper care is not given to mesh quality.

Table 2. Calculational Bias [% Difference between MCNP6.2 k-effective result and Experiment k-effective] and C/E [MCNP6.2 calculated k-effective/Experiment k-effective

Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
HEU-MET-FAST-001	0.00%	-0.16%	1.0000	0.9984
HEU-MET-FAST-007-037	0.30%	0.29%	1.0030	1.0029
IEU-MET-FAST-007	-0.01%	-0.05%	0.9999	0.9995
PU-MET-FAST-022	-0.17%	-0.40%	0.9983	0.9960
PU-SOL-THERM-001-001	0.58%	0.30%	1.0058	1.0030

The selected benchmarks represented in this report highlight a number of different mesh construction techniques concerning mesh quality for doing criticality calculations. In general, the MCNP UM geometry describes the boundaries of where material of a given type is located and through which radiation is tracked. For the purpose of computational performance, it is generally advantageous to keep the mesh size as small as possible while maintaining adequate representation shape of the material boundaries. For the purposes of modeling active assemblies, preserving mass as well as surface area to volume ratio to within 1-2% of nominal is crucial to getting k-effective results within 1% of the experimental results.

Other UM techniques considered in the mesh optimization process are:

- density adjustment to preserve critical mass,
- pre-faceting curved geometry, and
- homogenization of complicated parts.

Based on the results from the Godiva case shown HEU-MET-FAST-001, the density adjustment method should be used with care. If the density adjustment method is used it should be a small correction after the mesh has been converged to meet the volume and surface area/volume recommendations stated above.

The results for the Big Ten model demonstrated two other meshing strategies, namely pre-faceting and homogenization. Homogenization of fuel plates in the Big Ten model reduced the mesh size by over 50%, which resulted in substantial improvements in memory requirements, run time performance. Pre-faceting was also exploited in Big Ten where the control rods and cladding materials were pre-faceted using 20-sided polygons rather than keeping the true cylindrical geometry as shown in Figure 28. One advantage of the pre-faceted geometry rather than the true cylindrical geometry is that radial gap tolerances are strictly preserved all the way down the control rods for the pre-faceted geometry, but not for the true curved geometry with body fitted mesh. A second advantage, demonstrated in Figure 29, is that because no curvature needs to be resolved, the mesh size for the control rods may be substantially reduced.

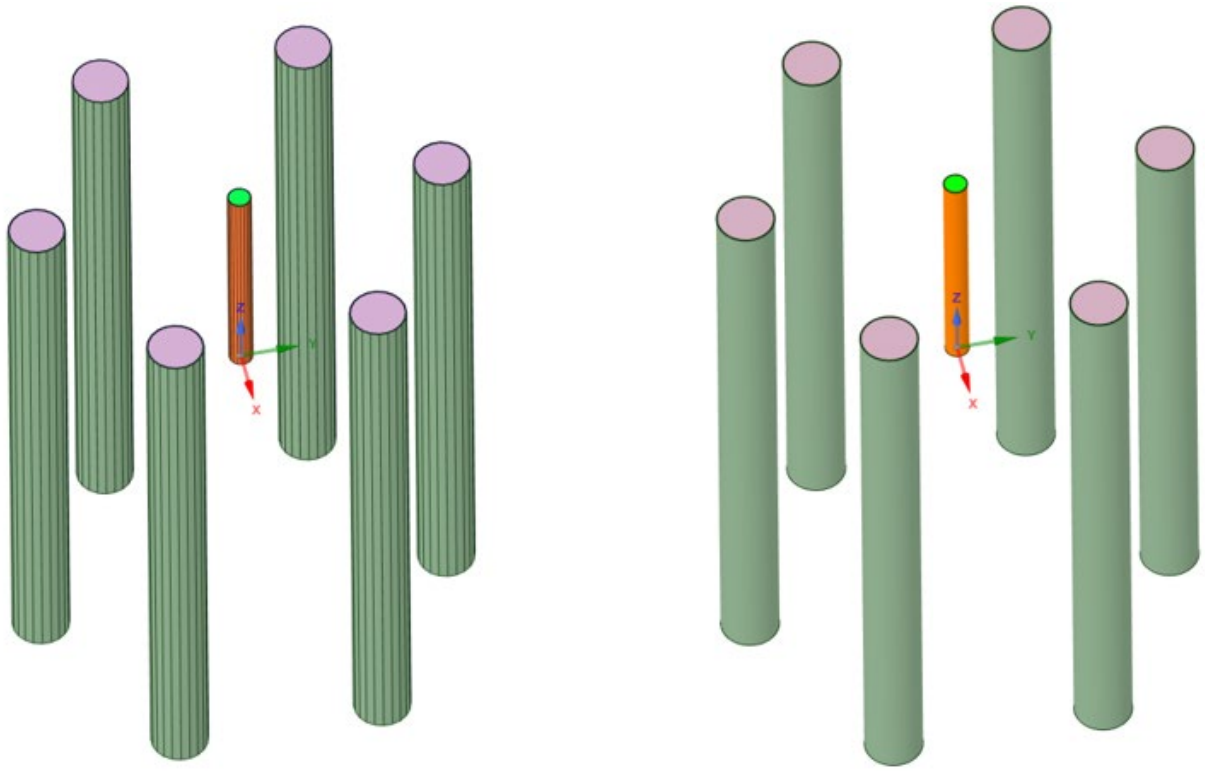

Figure 28. Pre-faceted Control Rod Geometry Compared to True Cylindrical Geometry

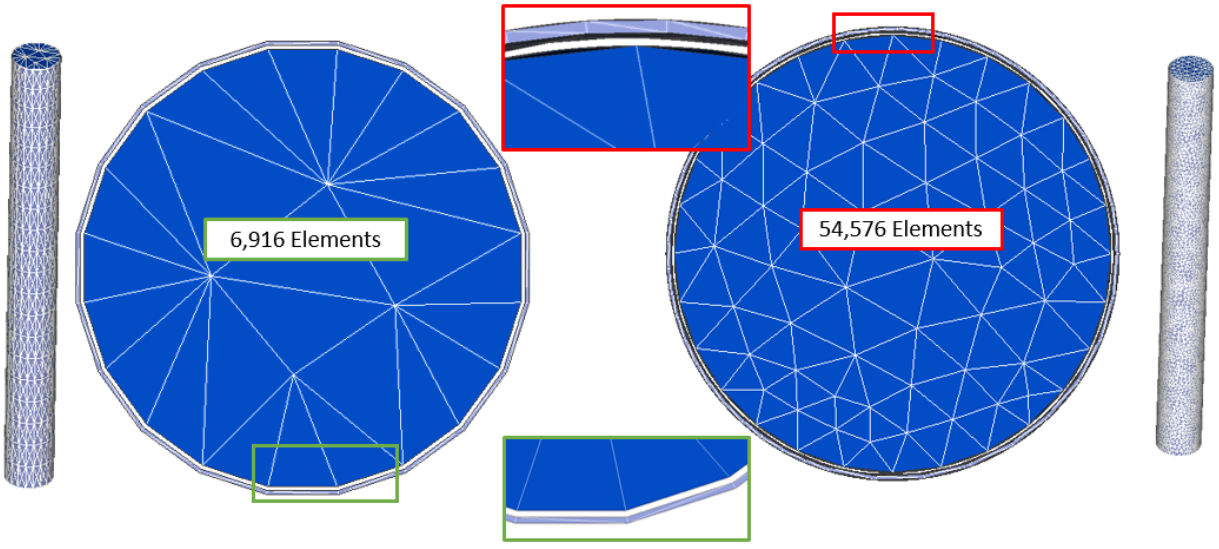

Figure 29. Comparison of Pre-faceted and True Cylindrical Geometry Post Meshing

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